

TITLE: THE INFLUENCE OF MOLECULAR STRUCTURE ON OLFACTIVE QUALITY (A QUANTITATIVE APPROACH)

AUTHORS: H. Boelens, H. G. Haring, and H. J. Takken*

AFFILIATION: Naarden International N.V., P.O. Box 2, Bussum, The Netherlands

ABSTRACT: Some investigations on the influence of molecular structure on the olfactive quality will be discussed. The influence of molecular structure on the olfactive quality of compounds with a fruity odor characteristic will be discussed in detail. More than 100 aliphatic, aromatic, and homocyclic esters were studied. We found in a quantitative approach of structure-odor relationship that (1) the steric parameter - aliphatic, arylepoxide, and homocyclic profile elements - have a significant influence and (2) the physicochemical parameters - molecular weight and partition coefficients - are non-significant over the whole group but they show some significance within subgroups.

REVIEW: The paper reports on the author's attempts to correlate chemical structures with odor. It is known that various classes of chemicals of similar structure frequently have similar and unique odors. However, this is not always the case and there are instances where materials of very different structure have similar odors and where comparable structures yield dissimilar properties. In addition, it is known that steric effects can have a marked influence on odor properties and that group replacement within molecules can yield similar odor characteristics. Regression analysis was used by the authors to try to quantitatively correlate structural features with odor characteristics. An equation was used in which 30 odor descriptors classified the materials investigated. The descriptors were taken from a master list of 300 chemicals with their individual odor descriptors.

$$\text{Olfactory quality} = \sum (\text{physicochemical parameters}) + \sum (\text{structural features}) + K$$

Thirty-five esters were chosen for the initial study to investigate their structures versus fruity odor. A relationship was found between the structures of the esters and this feature. This study was followed by one using 106 esters in which 91 were determined to have the fruity odor and 15 did not. A correlation with structure was also found in this study. A third investigation found a similar correlation with chain length of 34 aliphatic esters. The authors thus concluded that correlations do in fact exist between ester structure and fruity odor and that this correlation can be shown by the use of regression analysis.

-Reviewed by R. Comes.

1000816878